Cyclodextrin inclusion complexes with caffeoylquinic acids as bioactive compounds

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ABSTRACT: Neochlorogenic acid, a less-studied caffeoylquinic acid, isomer of chlorogenic acid, has been seen to possess antioxidant, antifungal, anti-inflammatory and anticarcinogenic effects, which makes it an interesting bioactive compound for incorporation in drugs, nutraceuticals or functional foods. However, its poor solubility in water and susceptibility to oxidation make such a task difficult. To overcome that, its encapsulation in cyclodextrins (CDs) is proposed. The fluorescence of neochlorogenic acid in different pH conditions was analyzed, and caffeic acid was proved to be the fluorescent moiety in the molecule. An encapsulation model whereby the ligand poses two potential complexation sites (caffeic and D-(-)-quinic moieties), showed that α-CD and HP-β-CD formed the best inclusion complexes with neochlorogenic acid, followed by M-β-CD, β-CD and γ-CD. Molecular docking with the two best CDs gave better scores for α-CD, despite HP-β-CD providing stabilization through H-bonds. The encapsulation of chlorogenic acid led to a similar CD order and scores, although constants were higher for α-CD, β-CD and M-β-CD, lower for HP-β-CD, and negligible for γ-CD. The solubility and the susceptibility to oxidation of neochlorogenic acid improved after complexation with α-CD and HP-β-CD, while the antioxidant activity of both isomers was maintained. These results could lead to obtaining more stable inclusion complexes with caffeoylquinic acids for applications in the pharmaceutical industry.

KEYWORDS: Neochlorogenic acid; Caffeoylquinic acids; Cyclodextrins; Encapsulation; Fluorescence

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